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MEMORANDUM FOR PRS (Contractor/In-House Publication)

FROM: PROI (TI) (STINFO) 08 February 2000

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2000-028**
Christe, K.O. (ERC), Zhang, X. (USC), Sheehy, J. (PRSP), Bau, R. (USC), "The tetrafluorohalogen cations ClF_4, SeF_4, and TeF_4"

American Chemical Society Mtg (San Francisco, CA, 26-30 Mar 2000) **(Statement A)**
(Deadline: 10 Mar 2000)

1. This request has been reviewed by the Foreign Disclosure Office for: a.) appropriateness of distribution statement, b.) military/national critical technology, c.) export controls or distribution restrictions, d.) appropriateness for release to a foreign nation, and e.) technical sensitivity and/or economic sensitivity.
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PHILIP A. KESSEL Date
Technical Advisor
Propulsion Science and Advanced Concepts Division

The tetrafluorohalogen cations ClF_4^+, BrF_4^+, and IF_4^+ and their isoelectronic counterparts SF_4, SeF_4, and TeF_4

Karl O. Christe[1], Xiongzhi Zhang[2], Jeffrey A. Sheehy[1], and Robert Bau[2]. (1) Propulsion Sciences and Advanced Concepts Division, Air Force Research Laboratory, Edwards Air Force Base, CA 93524, fax: 661-275-5471, karl.christe@ple.af.mil, (2) Department of Chemistry, University of Southern California, Los Angeles, CA 90089

The crystal structure of the 1:1 adduct, ClF_5SbF_5, was determined and shown to contain discrete ClF_4^+ and SbF_6^- ions. The ClF_4^+ structure can be described as a trigonal bipyramid with two longer more ionic axial bonds and two shorter more covalent equatorial bonds. The third equatorial position is occupied by a sterically active free valence electron pair on chlorine. The coordination about the chlorine atom is completed by two longer fluorine contacts in the equatorial plane resulting in the formation of infinite zigzag chains of alternating ClF_4^+ and -fluorine bridged SbF_6^- ions. Electronic structure calculations were carried out for the isoelectronic series ClF_4^+, BrF_4^+, IF_4^+ and SF_4, SeF_4, TeF_4, and their vibrational spectra and force fields were revised. A simple method was developed for modeling the effects of fluorine bridging on the individual ClF_4^+ and SbF_6^- ions in the infinite $-(ClF_4^+-SbF_6^-)-$ chains. This model can account for most of the discrepancies between the geometry and vibrational frequencies calculated for the free ions and those observed for solid $ClF_4^+SbF_6^-$.